NNDC Technical Support to the NCSP

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Cross Section Evaluation Working Group *(CSEWG)*

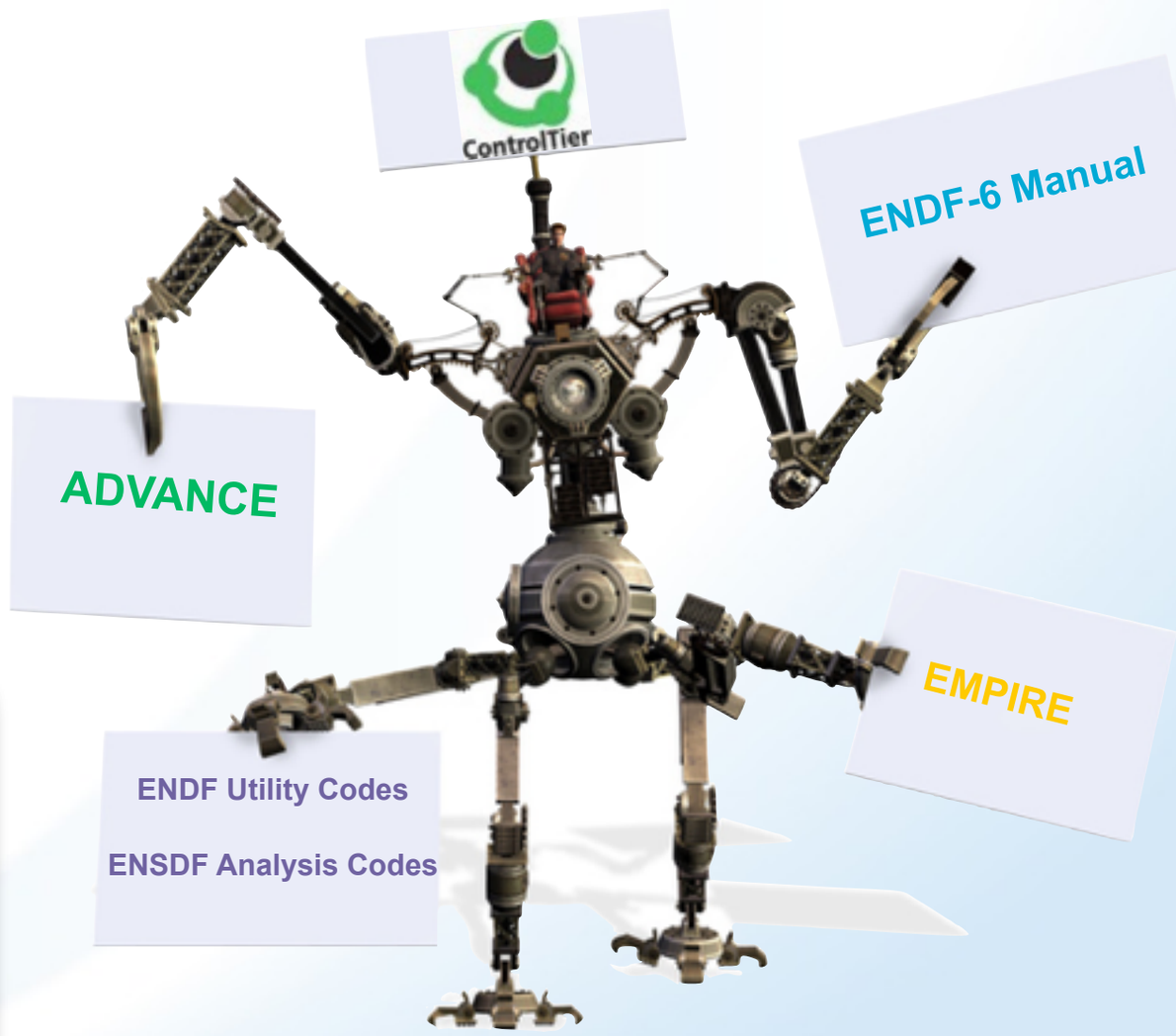
BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

2/3 of BNL's NCSP Nuclear Data tasks are now fully automated

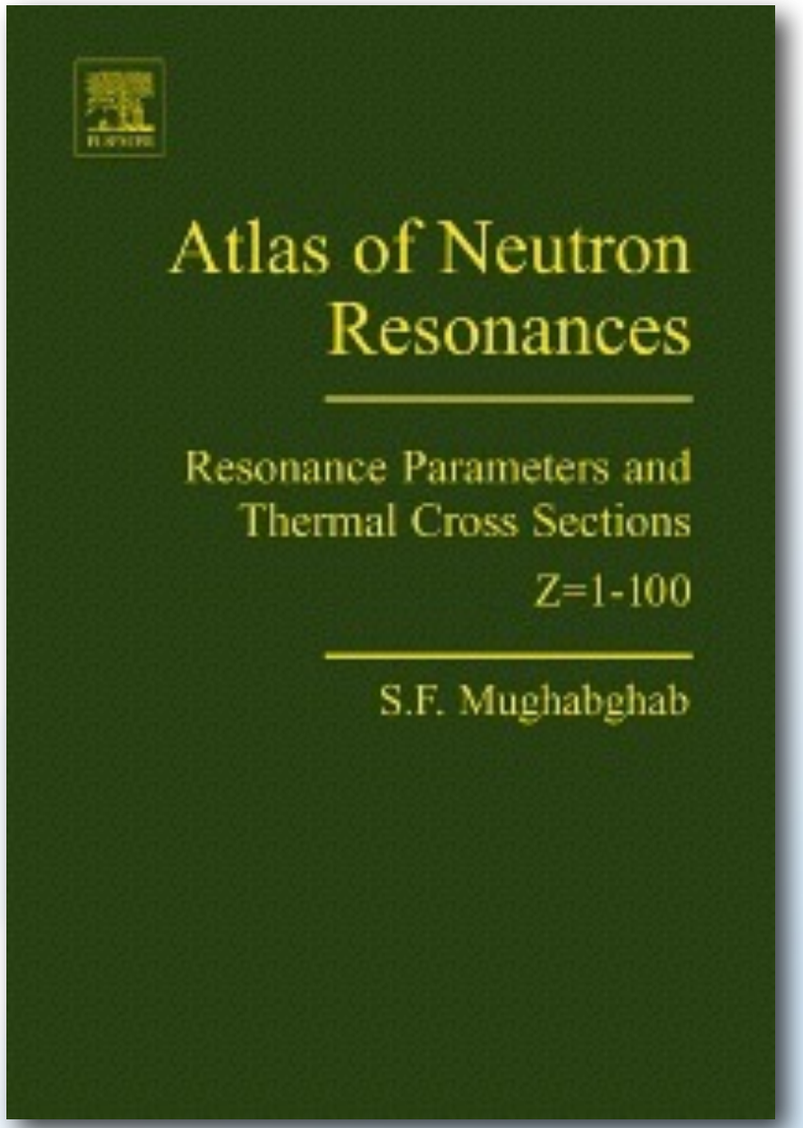
- ☑ **Perform data verification of new NCSP evaluations and store them on GForge server (Q1, Q2, Q3, Q4)**
- ☑ **Perform QA of new NCSP covariance data (Q2, Q4)**
- ☐ **Update Atlas of Neutron Resonances (Q4)**



Our scheme is so useful, in FY14, the NNDC has automated many other tasks with same system

The last task is on track

- ☑ **Perform data verification of new NCSP evaluations and store them on GForge server (Q1, Q2, Q3, Q4)**
- ☑ **Perform QA of new NCSP covariance data (Q2, Q4)**
- ☑ **Update Atlas of Neutron Resonances (Q4)**
  - **S. Mughabghab retired ~ 10 years ago so cannot charge NCSP**
  - **Integral parameters were updated and loaded into EXFOR database (#V1001)**
  - **Succession planning in progress in FY14**



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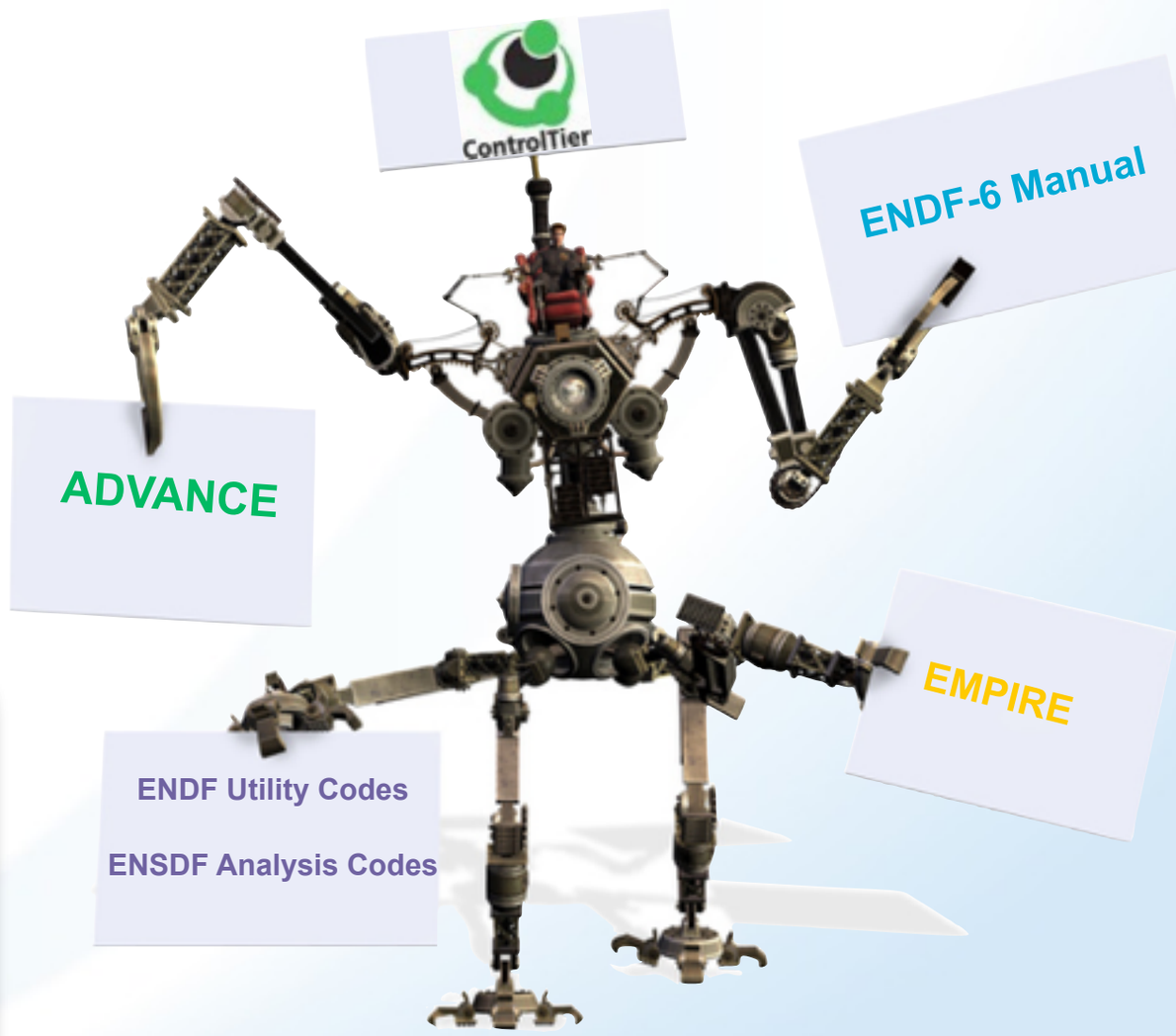
In the remainder of the talk, I want to tell you about the ADVANCE system



Benefits of automation are clear

- No waiting for assistance from processing code experts
- Extensive testing with minimum effort
  - Number of new commits verified
    - 1 deuteron-incident evaluation
    - 5 decay evaluations
    - 111 neutron-incident evaluations
- High-quality evaluations due to extensive and frequent testing
- Evaluation QA anywhere, anytime through Web at http://www.nndc.bnl.gov/endf/b7.dev/qa/
- Timely feedback on every change enables easier ID and correction of deficiencies

Expected Result

- Expedited submission of evaluations for CSEWG review
- Faster release of new evaluated data libraries

Why did we do it?

What's the Problem?

- Data verification and data validation (V&V) is tedious, so evaluators usually "forget"
- Not all evaluators know how to run the commonly used V&V codes
- Evaluators may have different versions (read: different bugs) of the same V&V code thereby producing different results

What's the solution?

- A highly automated, modular V&V system publicly accessible to evaluators

Automated Data Verification and Assurance for Nuclear Calculations Enhancement (ADVANCE)

Outline

- Motivation
- Benefits of ADVANCE
- The ADVANCE ND/QA System
  - ADVANCE System Architecture
  - ADVANCE Process Flow
  - Future Directions

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http://www.nndc.bnl.gov/endf/b7.dev/qa/index.html

ADVANCE: The ENDF Continuous Integration System

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ENDF B-VII.dev

ENDF/B Development

The development version of the Evaluated Nuclear Data File (ENDF/B)

Latest Updates

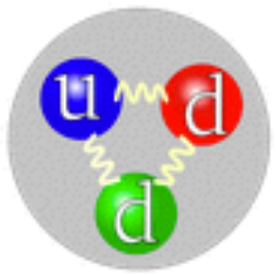
sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

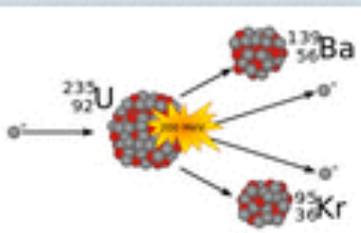
sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 15:41:29.746913

Neutrons | Decay | Charged particles | Photonuclear | Atomic

Neutrons sublibraries



Neutrons Sublibrary



Neutron-Induced Fission Yields Sublibrary

Standards Sublibrary

Thermal Neutron Scattering Sublibrary

Neutrons Sublibrary

ENDF/B Development Library

- General Information:
  - ENDF sublib designator: 10
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR
  - Build time: 2013-04-30 16:52:01.394282
  - Listfile: neutrons.list
  - Release Notes: neutrons-releaseNotes.pdf
- GForge Links:
  - Browse SVN
  - Browse sublibrary tracker

Latest Updates

sublib_release_notes: neutrons
Report sublib_release_notes on neutrons generated. The result was a SUCCESS
2013-04-30 16:57:39.661872

evaluation_summary: n-098_Cf_251.endf
Code evaluation_summary completed run on n-098_Cf_251.endf. The result was a SUCCESS
2013-04-30 16:52:41.503573

sublib_html: neutrons
Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

Periodic Table | Material List

1 H								X								2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe

- Build status: ERROR
- Build time: 2013-04-30 16:52:01.394282
- Listfile: neutrons.list
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Report sublib_html on neutrons generated. The result was a SUCCESS
2013-04-30 16:52:01.501892

- GForge Links:
  - Browse SVN

Pu

Status	Material	MAT #	Revision #	# Tests	# Failures	# Errors	Lab.	Date	Authors
	^{236}Pu	9428	603	756	0	44	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.
	^{237}Pu	9431	603	1398	0	136	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.
	^{238}Pu	9434	597	1004	0	180	LANL	SEP10	YOUNG, TALOU, KAWANO, KAHLER, CHADWIC
	^{239}Pu	9437	591	1508	0	68	LANL	SEP06	Young, Chadwick, MacFarlane, Derrien
	^{240}Pu	9440	532	1298	0	216	LANL	SEP09	YOUNG, TALOU, CHADWICK, KAHLER, KAWAN
	^{241}Pu	9443	532	924	0	10	ORNL	OCT03	L.Weston, R.Wright, H.Derrien , et al.
	^{242}Pu	9446	603	1268	0	108	BNL+JAEA	AUG11	S.F. MUGHABGHAB , et al. O.Iwamoto, etal
	^{243}Pu	9449	597	536	0	24	SRL,LLNL	JUL76	Benjamin, McCrosson, Howerton
	^{244}Pu	9452	603	846	0	60	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, , et al.
	^{246}Pu	9458	603	850	0	60	JAEA+	FEB10	O.Iwamoto, T.Nakagawa, et al.

* Lanthanides (Lanthanoids)	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
** Actinides (Actinoids)	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

2 He
10 Ne
18 Ar
36 Kr
54 Xe
86 Rn
118 Uuo

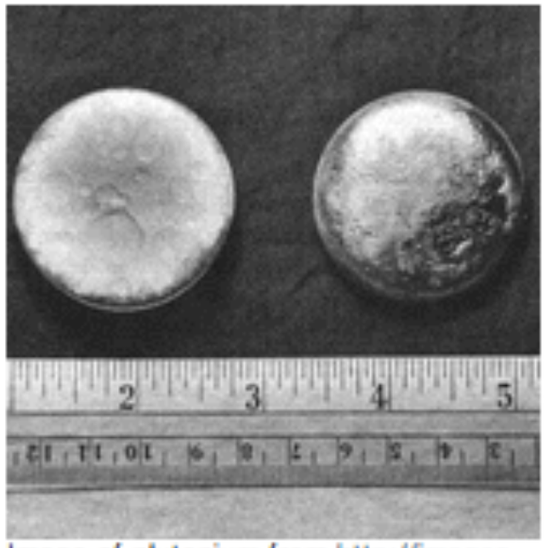


Image of plutonium from http://images-of-elements.com/

^{239}Pu

Neutrons Sublibrary

- General Information:
  - ENDF MAT designator: 9437
  - Evaluated by Young, Chadwick, MacFarlane, Derrien (LANL), SEP06
  - Natural abundance: 0.0 +/- 0.0 %
  - Check out Wikipedia's entry for plutonium
- Revision Number: 611M
- Last Modified Revision: 532:611M
- Build Status:
  - Build status: ERROR (Submit tracker item)
  - Build time: 2013-04-30 06:17:38.108808

- GForge Links:
  - Browse SVN
  - View current revision
  - Download current revision

Latest Updates

evaluation_summary: n-094_Pu_239.endf
Code evaluation_summary completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:17:39.392055

njoy2012: n-094_Pu_239.endf
Code njoy2012 completed run on n-094_Pu_239.endf. The result was a ERROR
2013-04-30 06:17:36.872836

inter: n-094_Pu_239.endf
Code inter completed run on n-094_Pu_239.endf. The result was a SUCCESS
2013-04-30 06:10:24.995505

Code Results | ENDF Overview | ACE Overview | Integral Quantities | Cross Section Plots

Summary of all tests on this evaluation.

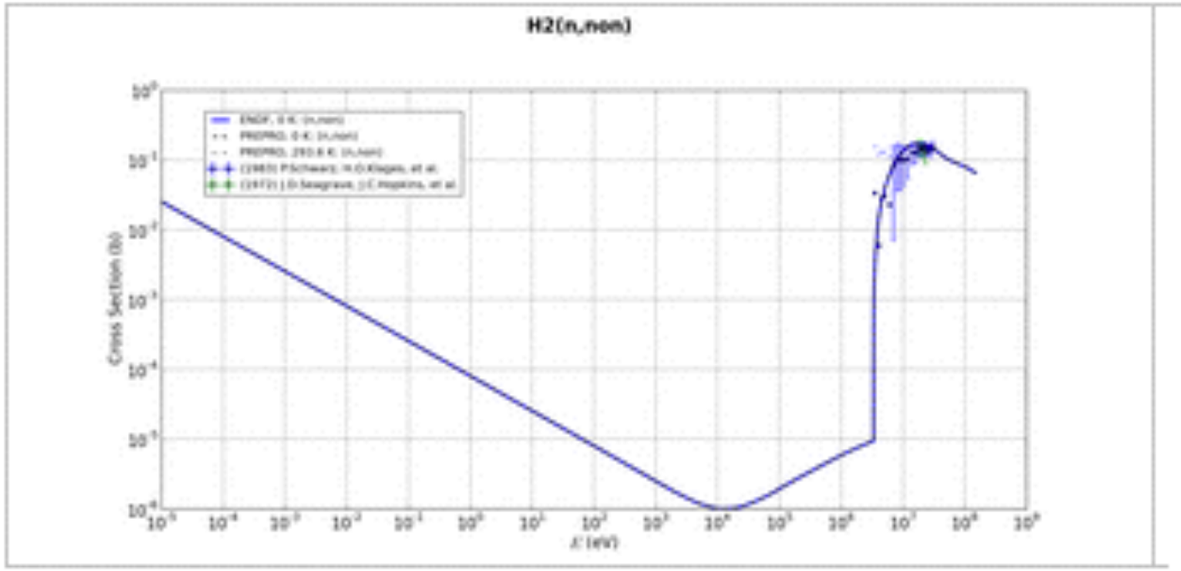
Use checking code button to show/hide errors.

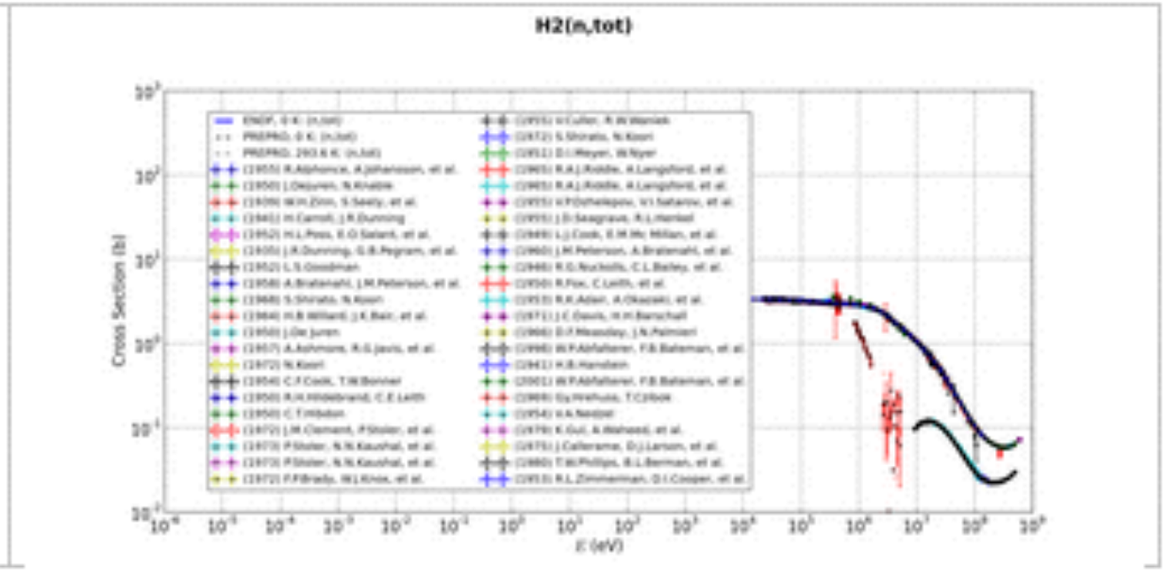
Status	Code	# Tests	# Failures	# Errors	Run time (sec)	Files
✓	STAN	0	0	0	31.533	STN File
✓	STANEF	0	0	0	29.316	

Code Results | ENDF Overview | ACE Overview | Integral Quantities | Cross Section Plots

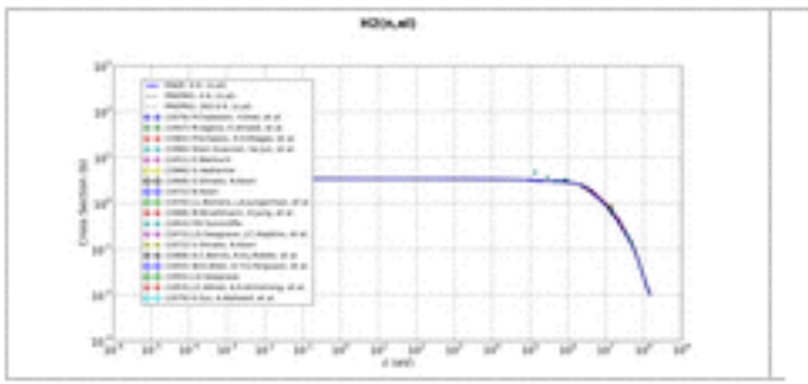
Comparison between cross section data in this ENDF file and data retrieved from EXFOR

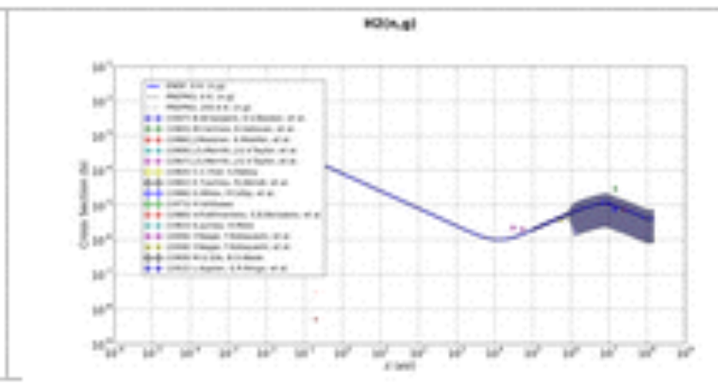
Aggregate channels:

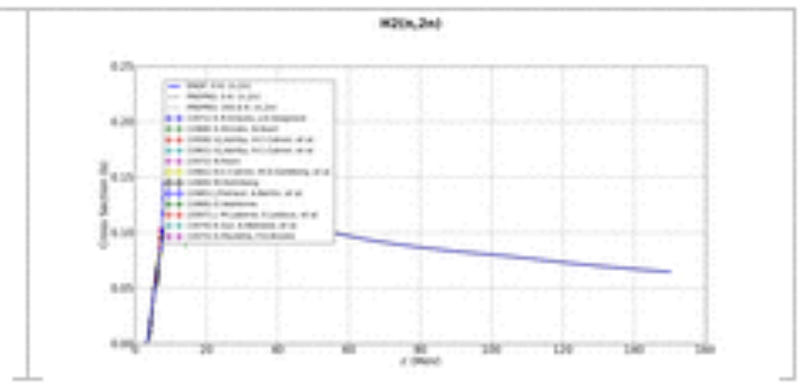




Regular channels:







ADVANCE Version 0.7 (svn rev: 669)

Codes used in ADVANCE version 0.7

- **NNDC checking codes**
  - STAN
  - STANEF
  - CHECKR
  - FIZCON
  - PSYCHE
- **PREPRO**
  - LINEAR
  - RECENT
  - SIGMA1
- **NJOY2012 (upgraded from NJOY99)**
  - grouping, heating, checking
  - ACE file
- **Fudge-4.0 (upgraded from Fudge-2.0)**
  - checking
  - cross section plotting
  - xml/html5 overview
- **Other Codes**
  - INTER: integral quantities
  - ACELST: ACE file overview
  - ENDF2HTM: ENDF overview
  - x4i: EXFOR data for plotting

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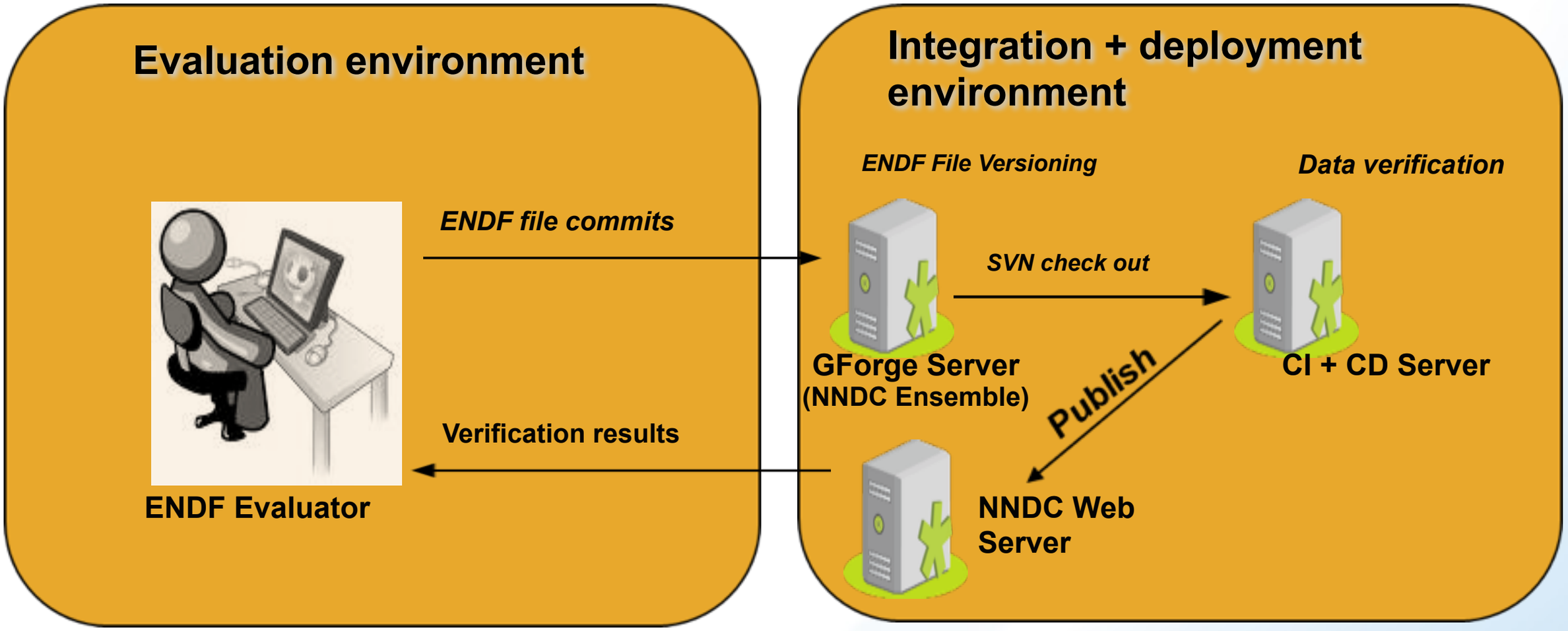
- ADVANCE Process Flow

Future Directions

ADVANCE System Architecture



- GForge Server as the versioning system (Subversion).
- Each commit to ENDF repository triggers data verification
- Results automatically posted on NNDC Web server

The ADVANCE ND/QA System (continued)

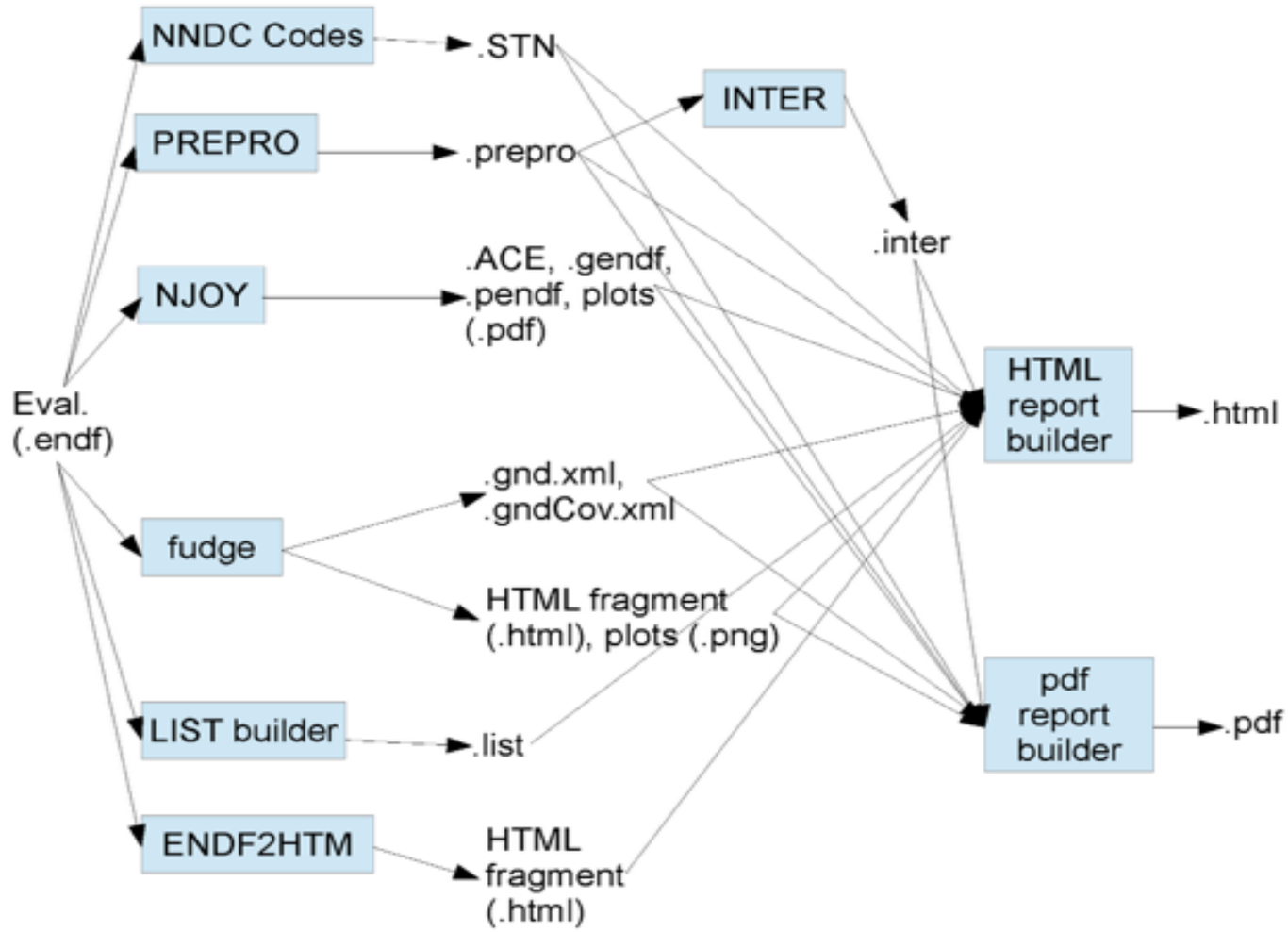
Why ControlTier?

- Robust and reliable
- Cost-free: Good for NNDC's tight budget
- Open-source: Can change system code
- Platform independent: 100% Java
- Most complete platform:
  - Continuous integration + continuous deployment
- Highly scalable: Add servers + clients as needed

ControlTier

ADVANCE Process Flow

Data Verification



Code Dependencies

- A code may depend on output of another code. Thus, a code may not begin processing until the immediate preceding code completes.
- If new commit does not modify input file to a code, then the code and its dependent codes are not executed.

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Automated benchmarking is one of NCSP's 5 year goals

Opportunities

- ***cnp_test_suite release***
- **Transport code and test suite donations**
  - ***COG release***
  - COG suite release
  - ***MCNP6 release***
  - Mosteller suite of 119 tests
  - BNL 1D Sn tests
- **NNDC cluster upgrade:** cluster size to double to 184 Intel Xeon nodes
- **ADVANCE master node upgrade**
- **NNDC webserver upgrade**

Challenges

- **Original ADVANCE server died in January**
- **ControlTier project ended:** in long term must switch control system to either RunDeck or BuildBot or similar

We developed a software requirements document, available at ENDF QA page: http://www.nndc.bnl.gov/endf/b7.dev/qa.html

Preparing for major ADVANCE update

ADVANCE System Requirements

ADVANCE System Requirements

Authors: David A. Brown, Ramon Arcilla, Michal Herman
National Nuclear Data Center
Brookhaven National Laboratory
Upton, NY 11973
Date: July 15, 2013
Revision: 3

0. Introduction

The NNDC requires a continuous integration/continuous deployment (CI/CD) system as part of its effort to automate and simplify our workload and to ensure software and data quality (especially for the ENDF/B series of nuclear data libraries [ENDF]). A continuous integration system is one that continually monitors a software repository (e.g. a subversion repository), extracts changes and builds and tests all changed components. A continuous deployment system takes the results of the integration step and publishes them to, for example, a website. CI/CD systems are a common tool for

Rest of FY14 plans for ADVANCE

- [x] **New Backend: BuildBot**
- [ ] **More reports**:
  - [ ] Plots of integral quantities (MACS, RI, Cf spect. ave.)
  - [ ] Better energy balance report
  - [ ] Covariance QA report
- [ ] **Full library tarballs** (ACE, gnd, gendf)
- [ ] **More processing codes:**
  - [ ] CALENDF
  - [x] Fudge improvements
  - [ ] NJOY improvements
- [ ] **Database of errors:**
  - [x] processing code error mining
  - [ ] regressions
- [x] **Notifications**
- [ ] **Help pages**
- [x] **Unit tests/docs**
- [x] **An ADVANCE paper will appear in ND2013 proceedings**
- [ ] **Open source release**
- [ ] **Prepare for benchmarking?**

By November 2014 Nuclear Data Week, CSEWG plans to tag ENDF/B-VII.2.β0

- Many fixes to neutrons to address issues uncovered by ADVANCE (NCSP)
- New Thermal Scattering Law data (SiO_2) from NCSU (NCSP)
- Many fixes to decay data from BNL planned (DOE-SC)
- $^{63,65}Cu$ from LANL is planned
- Zr from BNL is planned (DOE-SC)
- …

Acknowledgments

Many thanks to C. Mattoon (LLNL), B. Beck (LLNL), N. Summers (LLNL) and M.-A. Descalle (LLNL) for the advice and valuable assistance they provided especially at the early stage of the ADVANCE project and for providing us with LLNL's cnp_test_suite package.

D. Heinrichs and C. Lee for preparing COG for general release.